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APPLICATION OF NONLINEAR LEAST SQUARES
METHODS TO THE ANALYSIS OF SOLAR SPECTRA

John H. Shaw
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For the Period
June 1984 - June 1985

CALIFORNIA INSTITUTE OF TECHNOLOGY
Jet Propulsion Laboratory
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ABSTRACT

A fast method of retrieving vertical temperature profiles in the atmosphere and of determining the paths of the rays producing the ATMOS occultation spectra has been developed.

The results from one set of occultation data appear to be consistent with other available data.

A study of sources of error, a search for other suitable features for measurement in the spectra, and modification of the program to obtain mixing ratio profiles have been initiated.

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INTRODUCTION

One of the principal objectives of the ATMOS experiment is to obtain vertical mixing-ratio profiles (VMRs) of atmospheric gases. This requires the geometry of the ray paths and the vertical temperature and density profiles in the atmospheric region sampled. This information can be obtained from sources external to the experiment but its quality may not be sufficient to allow the highest accuracy in the VMR profiles of interest.

This information can be retrieved from the occultation spectra and we have demonstrated that temperature profiles and ray paths can be obtained from the ATMOS data quickly and precisely. However, in order to analyze all the available spectra, additional absorbing features must be identified and a thorough error analysis completed.

Descriptions of the method, the results and the current stage of error analysis are given.

METHOD

The analytical method has been described by Hoke and Shaw (Ref. 1). A series of suitable lines of gases with known vertical mixing ratios and with accurately determined line parameters are identified in the occultation spectra and their equivalent widths measured. In our retrieval of the temperature profile from sunset occultation number 6, obtained on April 30, 1985, up to 30 lines in sixteen spectra when chosen for analysis. These provided more than 120 equivalent widths. Some of these lines originated from low lying states and had temperature insensitive intensities. The equivalent widths of these lines allow the total amount of absorber along the path and hence in the ray path itself to be estimated (1). Another series of lines arising from high energy states was chosen because these lines intensities are strongly temperature dependent.

A nonlinear, least-squares (NLLS) program was then used to adjust the initial guesses for the temperature profile and the tangent heights of the rays until a best fit between the calculated and observed equivalent widths was obtained.

The parameters retrieved included the temperatures at fixed altitudes in the atmosphere and five parameters describing the dependence of the tangent heights of the rays on time.

In order to obtain a retrieval it is necessary to make numerous assumptions. These include:

1. The line parameters (intensity, position, shape, width, and lower state energy are accurately known.
2. The atmosphere is in hydrostatic equilibrium.
3. The VMR of CO_2 is known.

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4. There are no systematic errors in the equivalent widths.
5. The effects of winds can be included.
6. The effects of LTE/non LTE can be modelled.
7. Various smearing effects caused by the finite FOV of the instrument, by satellite motion, and by jitter in the sun tracker can be included in the analysis.
8. The atmospheric pressure at some reference altitude is known.

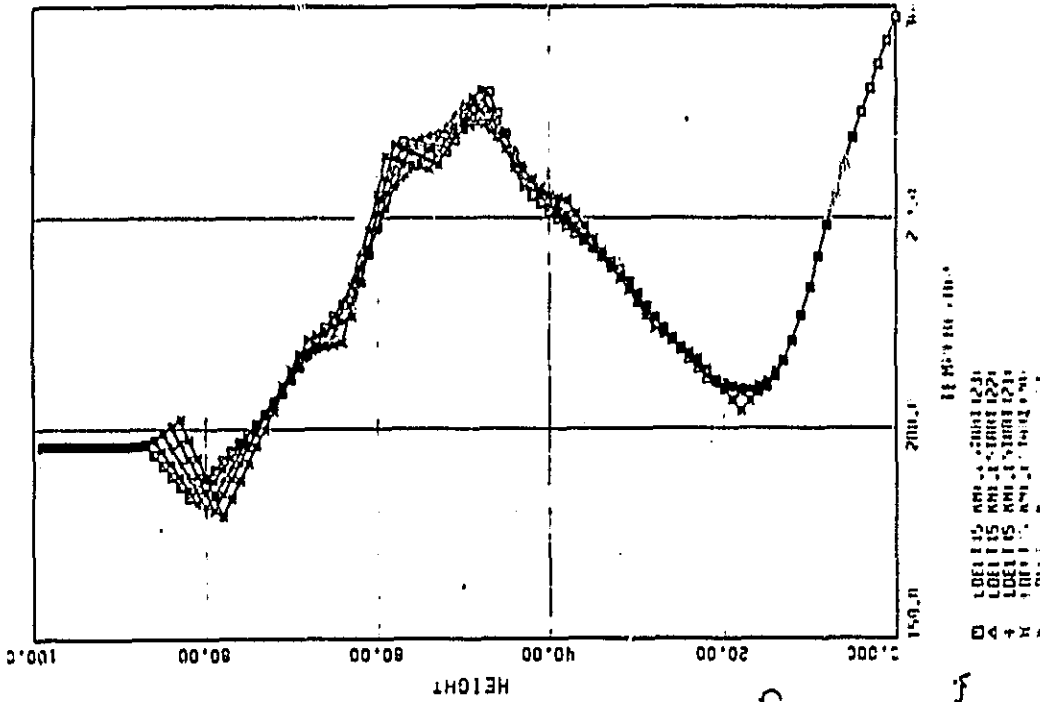
The effects of errors in some of these assumptions is discussed below.

RESULTS

The temperature profile in Fig. 1 was obtained by analyzing over one hundred equivalent widths of thirty lines of CO_2 occurring in sixteen spectra obtained during a sunset occultation observed by ATMOS on April 30, 1985.

The tangent heights of the rays lay between 15 and 85 km. Eleven temperatures at altitudes between 20 and 80 km were retrieved and these are compared with a temperature profile supplied by Oxford University in Fig. 1. By analyzing subsets of the data and by choosing different spacings and altitudes for the temperature parameters it has been shown that the observed features are reproducible.

Less than three minutes of computer time were required to obtain these results.



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Fig. 1a. Comparison of temperature profile obtained by using The Ohio State measured equivalent widths and retrieved program with the profile supplied by the Oxford group. In the OSU retrieval the temperature profile was constrained below 18 km and above 85 km.

b. The temperature profiles retrieved by using different heights for the temperature parameters.

SOURCES OF ERROR

Line Parameters

The lower state energies of all the CO_2 lines used in this work are accurately known and the use of equivalent widths does not require an accurate knowledge of the line positions. The doppler widths α_D can be calculated if the temperature is known. There are uncertainties in the line intensity S , the line shape, and the collision-broadened widths α_L .

Intensity Errors

The equivalent widths of the CO_2 lines analyzed do not lie in the linear region of the curve of growth. Since the lines have essentially a Voigt shape the variation of the equivalent widths on absorber amount is a function of α_D/α_L and hence of the height of the ray in the atmosphere. We have found that fractional errors $\Delta S/S$ of 5% in the temperature insensitive lines chosen cause errors in the estimated tangent heights of the rays of 0.4 km or less at all altitudes.

Fractional errors $\Delta S/S$ of 5% in the intensities of the temperature sensitive lines cause errors in the temperature profile which depend on E'' and on the position of the equivalent width on the curve of growth. For the lines chosen errors of less than 1K occur for lines with $E'' > 3000 \text{ cm}^{-1}$ but this increases to more than 3K for lines with $E'' \leq 800 \text{ cm}^{-1}$.

Line Widths and Shapes

Since $\alpha_D/\alpha_L \ll 1$ for lines formed above 50 km and since the lines chosen for measurement do not have significant contributions to the equivalent widths

from the Lorentz wings it is not expected that uncertainties in the collision broadened widths will significantly affect the results. It was found that increasing the width α_L by 20% changed the retrieved temperatures by less than 2K between 20 and 80 km altitude.

Volume Mixing Ratio

The CO₂ volume mixing ratio is well known below 60 km. At higher altitudes dissociation occurs and there is considerable uncertainty in this VMR profile.

We have found that a change of 2% in the CO₂ VMR causes changes of less than 0.2 km in the retrieved tangent heights and the change in the temperature profile is less than 1K. Much larger uncertainties in the VMR above 60 km are anticipated. In this case it may be necessary to assume the ray paths are known and to retrieve the temperature and VMR (CO₂) simultaneously. We have not yet explored this problem in depth.

Reference Pressure

In order to describe the ray paths through the atmosphere, obtained from the spectra, in terms of the geometry of the occultation, it is necessary to assume that the atmospheric pressure at some reference altitude is known. This problem has been discussed by Shaffer et al (2) who have shown that a fractional error $\Delta P/P$ of 5% in the reference pressure causes a corresponding change in the tangent heights of the rays of less than 0.5 km.

However, errors in the tangent heights of the rays introduce errors in the temperature profile. We have found that an error in the tangent height of 1 km, which corresponds to an error in the reference pressure of 10%, causes

an error in the temperature parameters which increases with height above the reference pressure level from about 3K/km near 30 km to 6-7 K/km near 80 km.

Winds

Variations in the component of the wind along the line of sight and at different levels in the atmosphere cause line shifts. These shifts are small but should be observable in the ATMOS spectra (see Appendix A). Provided the lines are in the linear region of the curve of growth these wind speed changes will not alter the equivalent widths of the lines. However, as the lines saturate, wind speed differences cause the observed equivalent widths to increase. We have found that, provided the wind speed is less than 100 m/s the maximum fractional increase in the equivalent width $\Delta W/W$ is less than 3% at all heights and at all frequencies. This is only slightly larger than the estimated uncertainty in measuring the equivalent widths of the lines and is therefore not considered to be an important effect.

Spectral Smearing

Because of satellite motion during the period of data collection, the finite field of view (FOV) of the instrument, and jitter in the sunseeker the collected spectra are some weighted mean of many atmospheric paths. For a 2mr FOV these effects are equivalent to a spread in the tangent heights of the rays reaching the instrument of more than 6 km. If spectra are averaged this spread is increased.

These effects limit the vertical resolution of the temperature and VMR profiles and they may also affect the accuracy of the retrieved profiles unless they are included in the data analysis. In particular, if there is a

significant vertical temperature gradient over the FOV then the absorber-mass-weighted mean tangent height determined from the pressure lines may differ from the line-intensity-mass-weighted mean tangent height of the temperature sensitive lines. These effects have not yet been thoroughly explored. It is expected that some method of weighting for these effects must eventually be included in the calculations. One method is evaluate mean spectra by considering the contributions of several ray paths to each spectrum.

Non-LTE Effects

Departures from LTE are expected to occur in the atmosphere above about 50 km. We have not yet included these effects in our calculations or considered uncertainties in these effects on the retrieved temperature profiles.

Sensitivity

In the previous section we have discussed the effects of systematic errors in the assumed models and model parameters on the retrieved temperature profiles. We have found, by changing these models and model parameters, that significant changes in the retrieved vertical temperature profiles can be made.

However, in all the cases we have explored, it has been found that the solutions are strongly convergent and that the final profiles are obtained after only a few iterations.

Although, we expect significant effects due to improvements in the CO₂ VMR and to the inclusion of non-LTE effects in the temperature profiles obtained at 100 km and above it appears that the precision with which most of the other required parameters is already known is sufficient to obtain

temperature profiles accurate to 2-3K and hence that the principal source of uncertainty is due to the information content of the spectra.

This information is limited by the SNR of the collected spectra, by the frequency spacing of the spectral data, by the finite instrumental resolution, and by the necessity for using partially saturated lines, since the equivalent widths of lines in the linear region of the curve of growth are too small to be measured accurately.

For lines in the linear region of the curve of growth the ratio $(\Delta W/W)/(\Delta u/u)$ when u is the absorber amount is unity. The corresponding value of this ratio for the CO_2 lines measured in this study was, in some cases, as low as 0.2.

Despite this lack of sensitivity and the measurement precision of about 2% in the equivalent widths the precision of a few degrees in the retrieved temperature profile is excellent at this stage in the analysis.

Summary of Systematic Error Effects

These estimates are based on the analysis of simulated data similar to those obtained from ATMOS occultation SS06.

Effect	Magnitude of error	Effect on h_T	Effect on T profile
Measurement of equivalent width	$\Delta W/W = 5\%$	< 0.7 km	1.5 - 5K
Line Intensity	$\Delta S/S = 5\%$	< 0.5 km	1 - 3K (depends on E'')
Collisional width	$\Delta \alpha/\alpha = 20\%$	< 0.5 km	< 2 K
Volume mixing ratio	$\Delta(\text{VMR})/\text{VMR} = 2\%$	< 0.2 km	< 1 K
Pressure at reference altitude	$\Delta P/P = 5\%$	< 0.5 km	3 - 8K
Winds	$\Delta W/W < 3\%$ for $v = 100$ m/s	< 0.4 km	1 - 3K
Spectral smearing		< 0.5 km	1.5 - 4K
LTE/Non-LTE		to be investigated	

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APPENDIX

Atmospheric Winds from Occultation Spectra*

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Abstract

By measuring the mean shifts of hundreds of lines in solar occultation spectra obtained at satellite altitudes relative wind speeds along the lines of sight of the rays can be obtained with precisions of 5 m/s or better at altitudes up to 100 km. It is necessary to obtain more accurate line positions or to introduce a gas sample for frequency calibration if absolute wind speeds are to be obtained.

Introduction

A series of solar occultation spectra is expected to be obtained with a Fourier Transform Spectrometer* carried on the Space Shuttle. This ATMOS instrument collects spectra in broad regions between 2 and 16 μm at a rate of about one per second and with a spectral resolution of about 0.01 cm^{-1} as the tangent heights of the rays vary from 0 to over 150 km. Solar lines occur in spectra of large tangent heights and, as the rays penetrate more deeply into the atmosphere, thousands of lines belonging to more than thirty atmospheric gases are also formed. Many of these lines are due to CO_2 which has strong bands near 2.0, 2.7, 4.3 and 15 μm . Some lines of CO_2 appearing in a simulated spectrum with a resolution of 0.01 cm^{-1} and a tangent height of 85 km are shown in Fig. 1.

Because of the relative speeds v of the satellite with respect to the undisturbed solar atmosphere or the earth's atmosphere along the lines of sight of the rays the spectral features are shifted by amounts $\Delta\nu$ where

$$\Delta\nu/\nu = v/c. \quad (1)$$

These shifts can be calculated from the orbital geometry parameters.

Atmospheric motions or wind components along the line of sight introduce additional line shifts. By measuring these shifts as the FOV moves over the solar disk information about motions in the solar atmosphere can be obtained. Winds of up to 100 m/s occur in the earth's atmosphere. These speeds vary with altitude and location and hence telluric lines with contributions from different levels in the atmosphere may have distorted shapes and shifts.

*The ATMOS instrument is primarily intended for investigating the composition of the stratosphere and mesosphere. The principal investigator is C. B. Farmer of the Jet Propulsion Laboratory.

Useful meteorological information can be inferred if the wind speed components along the line of sight as low as 5 m/sec (10 mph) can be measured. These components are described as winds in the remainder of this discussion where it is shown that these precisions can be achieved if the instrument is stable.

The wind information obtained from the ATMOS spectra has a high vertical resolution over the region from below 30 km to above 90 km. A number of other methods for determining winds in this region by satellite remote sensing have been proposed. All are based on detecting the effects due to Doppler shifts and they have been summarized or referenced in papers by Reese (1), Hays (2), and McCleese and Margolis (3). Some techniques (1,2) measure the shift of a single line observed with a high resolution Fabry-Perot interferometer or the combined effects due to many lines as measured with a non-dispersive instrument (3). The precision of the method discussed below is enhanced by the measurement of the mean shifts of hundreds of lines.

Line Shapes and Shifts

Most absorption lines in the earth's atmosphere can be described by the Voigt shape. In the troposphere this approaches the Lorentz shape with typical widths of somewhat less than $0.1 \text{ cm}^{-1}/\text{atm}$. Above the tropopause the shape approaches the Doppler shape and the widths are given by

$$\alpha_D/v = 7.16 \times 10^{-7} (T/M)^{1/2},$$

where T is the temperature and M is the molecular weight of the absorber.

Over the range 0 to 100 km atmospheric temperatures vary from about 200 to 300 K and the molecular weights of many absorbing molecules lie in the range from about $M = 16$ (CH_4) to $M = 44$ (N_2O , CO_2). Doppler widths for several sets of values of T and M over the region from 500 to 5000 cm^{-1} are given in Table 1.

The Doppler shifts caused by winds of 5 m/s and 100 m/s over this same region are shown in Table II. These shifts are small compared with the line widths in Table I and also with the resolution R of about 0.015 cm^{-1} of the apodized (4) ATMOS spectra. Hawkins et al (5) have found that the positions of lines with widths narrower than the spectral resolution, observed in Fourier transform spectra with SNR's in excess of 100 can be estimated with precisions of $R/30$ or better. The ratios $P = 30\Delta v(5 \text{ m/s})/R$ in Table II show that, with this criterion, the minimum wind speed of 5 m/s cannot be estimated from a single line. However, the required precision can be achieved by measuring $N = 1/P^2$ line positions (5). The value of N in Table II increase rapidly as the line frequency decreases because the Doppler shift is directly proportional to frequency.

The shifts caused by a 5 m/s wind are smaller than the accuracies with which the frequencies of many lines of gases such as CO_2 , H_2O , N_2O , CO , or CH_4 are known (3). Thus, although it is possible to measure the relative shifts of groups of lines due to winds in different spectra, and hence to obtain the relative wind speeds, the determination of the absolute wind speed from the spectra requires additional spectroscopic measurements. Until these are available it will be necessary to normalize the relative wind speeds by direct comparison with in situ wind measurements.

Choice of Lines

The lines occurring in the spectra include:

1. Solar lines. These appear in all the spectra but many are obscured by telluric lines at low tangent heights. These solar lines do not yield direct information about motions in the earth's atmosphere. However, by measuring the relative shifts of groups of lines observed in successive spectra of large tangent heights, the short term stability of the

instrument and the guiding accuracy of the sunseeker can be inferred. The changes in the relative speed of the satellite and the solar atmosphere over the portion of the solar disk viewed can also be determined.

2. Lines of stratified atmospheric gases. Some gases such as O_3 have strongly peaked mixing-ratio profiles and produce large numbers of measurable lines in the spectra. Below some critical height the peak absorptances of these lines increase until the layer of maximum concentration is penetrated. If this increase is sufficiently rapid the wind-induced shifts of the lines in each spectrum are dominated by the winds in the lowest layer penetrated. Also, if there is little absorber in the atmosphere below the concentration maximum, the peak absorptances of the lines in spectra obtained for lower tangent heights no longer increase and the wind shifts are frozen. Such lines can be used as markers with which new lines of other gases appearing in spectra below this peak can be compared.

3. Lines of gases with nearly constant mixing ratio profiles. Although the peak absorptances of lines of gases such as CO_2 depend on the line intensity and spectral resolution they all increase steadily as the tangent height decreases. An example of this growth for a line of a gas with a constant mixing-ratio in the standard atmosphere is shown in Fig. 2. The dependences of the peak absorptances of other lines with different intensities on tangent height are shown in Fig. 3. Since line positions can usually be most precisely measured if the peak absorptances lie in the range 20 to 80% these curves indicate that each line can be used over a range of about 20 km and that several sets of lines are required to cover the region of interest.

Estimation of Wind Speeds from Lines of a Gas with a Constant Vertical Mixing-Ratio

The relative velocity of the satellite and the "wind free" atmosphere is essentially the same for all the molecules along the atmospheric path and thus it produces the same shift for all the "components" of the line formed in the 30 km deep layer where most of the absorption occurs. Uncertainties in the satellite height of 10 km or of 1° in the latitude of the closest approach of the ray to the earth cause errors of less than 5 m/s in this motion. Since the orbital parameters are known to this accuracy or better the shift due to satellite motion can be accurately calculated and the absolute wind speeds can be obtained from the residual shift, provided the absolute frequencies of the lines are known.

If the entire atmosphere above some level h_1 has a wind speed v_1 then all the components of a line in spectrum S_1 observed for rays with a tangent height h_1 are wind shifted by

$$\begin{aligned}\Delta v_1 &= v_1 - v_0, \\ &= v_1 v_0/c, \end{aligned} \quad (2)$$

where v_0 is the position of the line in the absence of a wind and $\Delta v_1 \ll v_0$. The contributions by the absorber above h_1 to the same line in spectra with lower tangent heights will also be shifted by Δv_1 . In spectrum S_2 , obtained for a ray path with a tangent height $h_2 = h_1 - \Delta h_2$, the same line has an increased peak absorptance due to the absorber Δu_2 along the path in the layer Δh_2 . If there is a wind v_2 in this layer the contribution to the line by Δu_2 in spectrum S_2 and other spectra with tangent heights less than h_2 is shifted by

$$\begin{aligned}\Delta v_2 &= v_2 - v_0, \\ &= v_2 v_0/c.\end{aligned}$$

Above 30 km lines which are not strongly saturated have shapes which are nearly invariant with height and the net shift δv_2 of the observed line in spectrum S_2 with respect to v_0 can be considered, to a first approximation, as the mean of the line shifts weighted by the amounts of absorber above and below h_1

$$\delta v_2 \approx (\Delta u_1 v_1 + \Delta u_2 v_2) v_0 / (\Delta u_1 + \Delta u_2) c.$$

In general

$$\delta v_n \approx (v_0/c) \sum_{i=1}^n \Delta u_i v_i / \sum_{i=1}^n \Delta u_i.$$

If, for example, all the winds are zero except in the bottom layer Δh_n the shift

$$\delta v_n = (v_0/c) \Delta u_n v_n / u,$$

where

$$u = \sum_{i=1}^n \Delta u_i.$$

Hence

$$\delta v_n / \Delta v_n = \Delta u_n / u. \quad (3)$$

As the thickness Δh_n increases Δu_n increases and $\delta v_n \rightarrow \Delta v_n$. Although the line shift can be measured more precisely the vertical resolution decreases.

When $\Delta u_n = u/2$ the ratio of the shifts in Eq. 3 is 0.5. The change in tangent height required to double the amount of an absorber, with a constant vertical mixing-ratio, along the ray path varies from about 4.5 to 5.5 km over the altitude range 0 to 100 km. Thus, if it is desired to obtain the winds in layers 5 km thick by measuring the shifts of CO_2 lines, these shifts are approximately one half those given by Eq. (2) and four times the number of lines given in Table II must be measured to obtain a precision of 5 m/s.

Inspection of lists of the parameters of atmospheric lines and of simulated solar spectra such as that in Fig. 1 indicates that there are sufficient numbers of strong lines near 2.7 and 4.3 μm to allow winds to be measured up to 100 km.

Discussion

It has been shown that winds speeds can be determined with accuracies of 5 m/s from ATMOS spectra provided the orbital parameters, and the line positions are accurately known and the instrumental performance is reproducible. Ground based tests have indicated that the instrument is stable and the stability in orbit can be confirmed by measuring the positions of solar lines. These solar lines can be used to transfer the frequency calibration from one spectrum to another provided that motions in the solar atmosphere are small. In future experiments the system can be internally calibrated with the method described by Hawkins et al (5) by introducing an absorption cell containing a mixture of absorbing gases.

The number of lines to be measured to obtain the desired precision is only a small fraction of the total number of observable lines. Indeed the reproducibility of the results can be compared by measuring the mean shifts of subsets of lines selected on the basis of their peak absorbance, origin, separation from other lines, etc.

In this discussion it has been assumed that the line shape is invariant with height and that the mean line shift is the mass weighted shifts of the individual layers. Better estimates of the relations between the observed mean line shifts and the wind speeds can be obtained by computer simulations. Synthetic spectra covering wide spectral regions and incorporating the effects of winds, spectral resolution, finite FOV, and satellite motion can be calculated if the tangent heights of the rays, the molecular line parameters

including the positions, intensities and shapes and the atmospheric characteristics such as the vertical pressure, temperature and absorber mixing-ratio profiles are known (7). If necessary, the effects of pressure shifts of the lines can be included although McCleese and Margolis (3) note that this effect should be negligible above 40 km.

Even though the vertical resolution is high the amount of information which can be obtained from occultation spectra is limited by the low spatial resolution caused by the long atmospheric paths and because each of the recorded spectra samples a different portion of the atmosphere. Thus only mean values of the atmospheric properties such as temperature, absorbing mixing-ratio or wind speed can be inferred.

In addition to affecting the line positions wind shears may also affect the shapes and the equivalent widths of the lines. Since most lines which are observed in spectra with tangent heights above 30 km and which have absorptances of 20% or greater lie outside the linear region of the curve of growth, the differential line shifts will increase the observed equivalent widths. The effects caused by most of the winds encountered in the atmosphere are not likely to introduce significant errors in, for example, the determination of the vertical mixing-ratios of trace gases. These effects may, however, limit the accuracies with which isotopic abundances can be determined and also the pressure or temperature profiles derived from the spectra. Most of the methods for inferring these profiles are based on the differences in the behavior of lines with temperature sensitive and insensitive intensities and are strongly dependent on the ability to fit the observed absorption accurately. Under some circumstances it may be necessary to retrieve the wind field simultaneously with the temperature profile.

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Table I

Range of Doppler widths of lines of
atmospheric molecules between 0 and 100 km

T(K)	M	$10^3 \alpha_D \text{ (cm}^{-1}\text{)}$		
		$\nu = 500 \text{ cm}^{-1}$	$\nu = 2000 \text{ cm}^{-1}$	$\nu = 5000 \text{ cm}^{-1}$
200	44	0.8	3.0	7.6
250	30	1.0	4.1	10
300	18	1.5	5.8	15

Table II. Wind induced Doppler shifts, and the numbers of line positions required to measure 5 m/s winds

Wave-number (cm^{-1})	Doppler Shift $\Delta\nu(\text{cm}^{-1})$		Resolution $R(\text{cm}^{-1})$	$P = \frac{30\Delta\nu(5 \text{ m/s})}{R}$ R	No. of lines $N = 1/P^2$
	$v=5 \text{ m/s}$	$v=100 \text{ m/s}$			
500	2×10^{-6}	1.7×10^{-4}	0.015	0.016	4000
2000	3×10^{-5}	6.2×10^{-4}	0.015	0.06	280
5000	8×10^{-5}	1.7×10^{-3}	0.015	0.16	40

Figure Captions

- Fig. 1 Absorption by CO_2 in a simulated occultation spectrum with a resolution of 0.01 cm^{-1} and a tangent height of 85 km.
- Fig. 2 Simulated spectra of a line of a gas with a constant vertical mixing-ratio observed with a resolution of 0.015 cm^{-1} and tangent heights of 43, 47, 51, and 55 km.
- Fig. 3 The dependence of the peak absorptance of lines of a gas with a constant vertical mixing-ratio on tangent height. These values were obtained from simulated spectra with a resolution of 0.015 cm^{-1} and the intensities of the lines change by a factor of 10 in successive curves. The topmost curve corresponds to one of the stronger lines of CO_2 near $15 \mu\text{m}$.

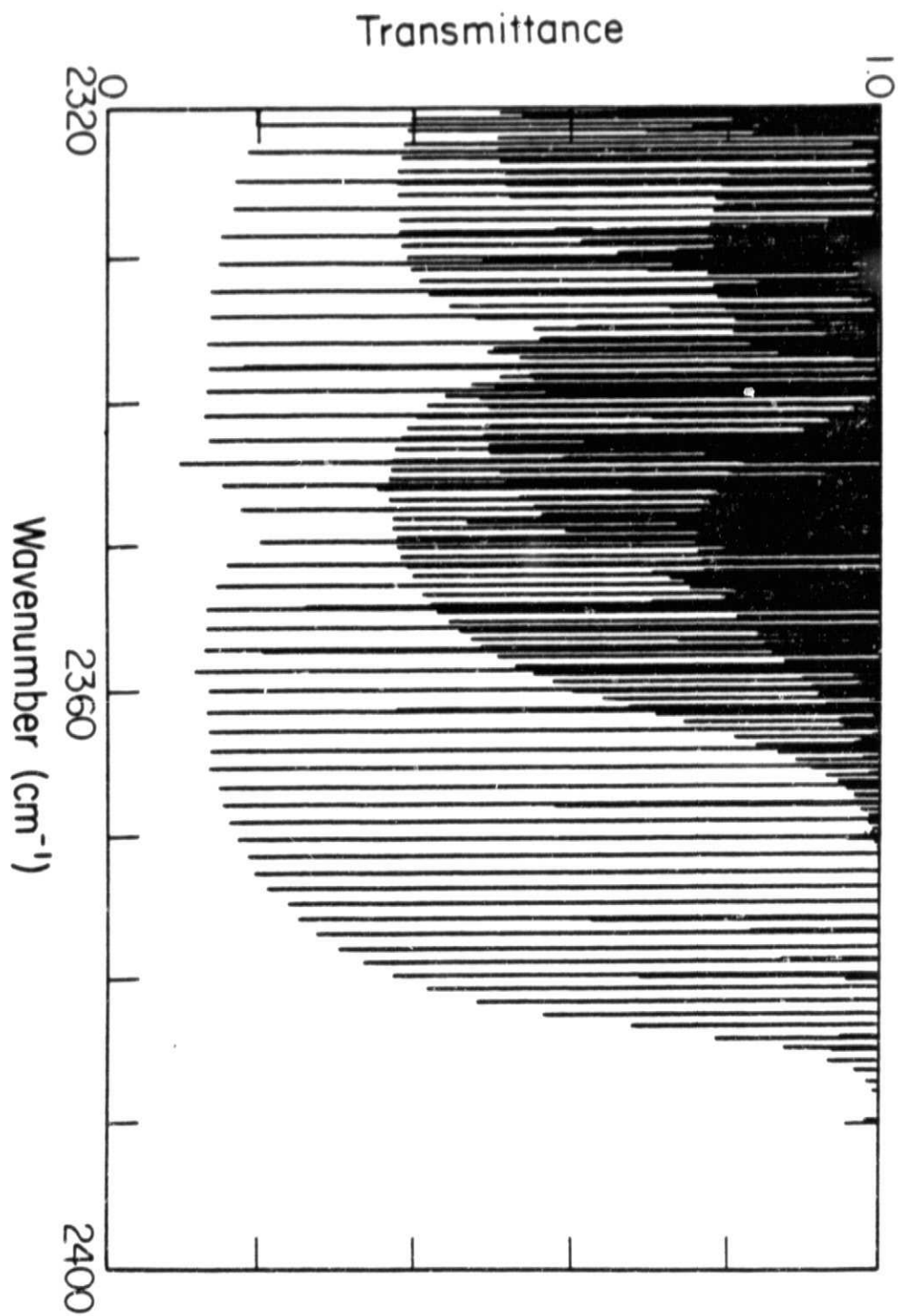


Fig. 1

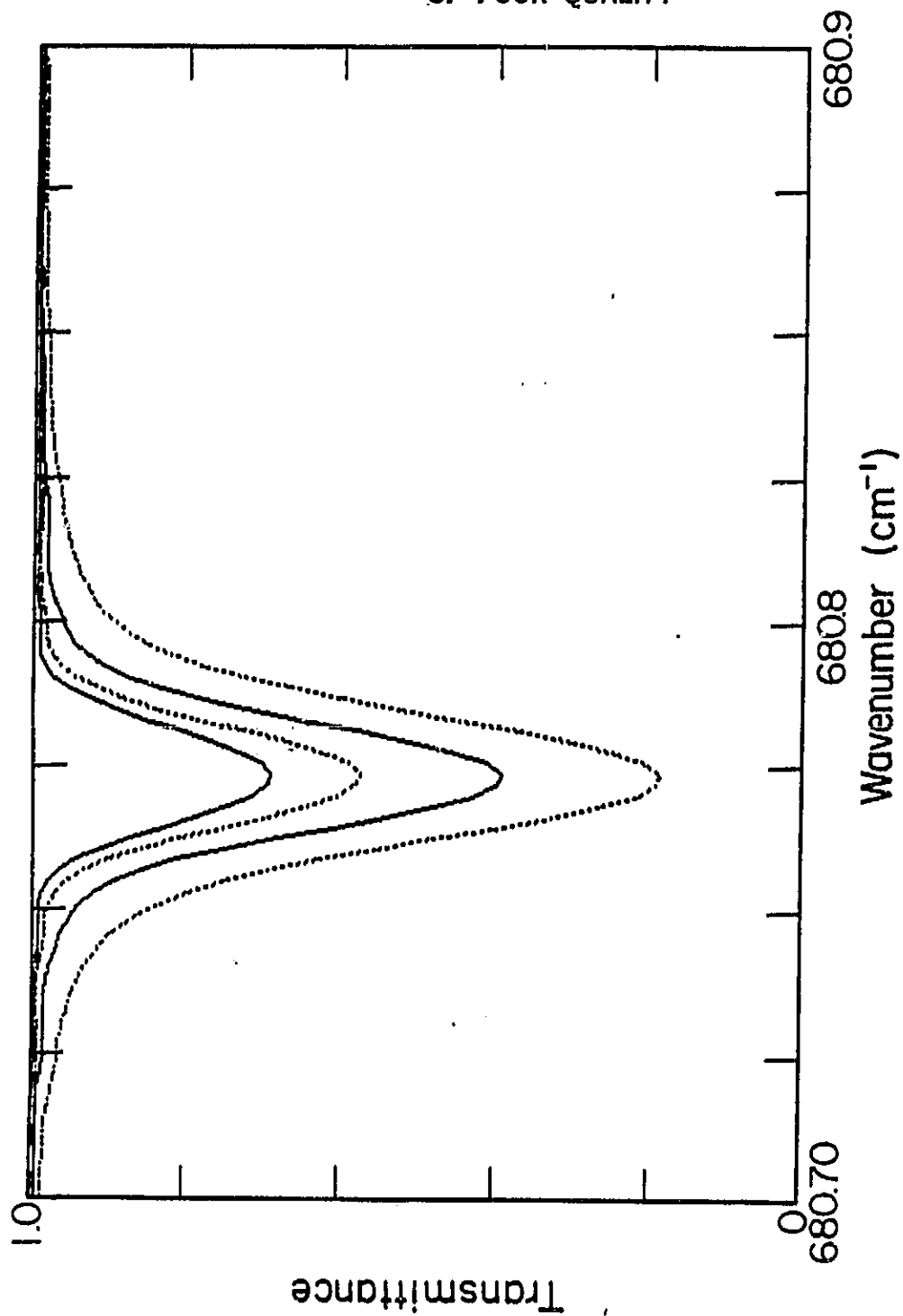


Fig. 2

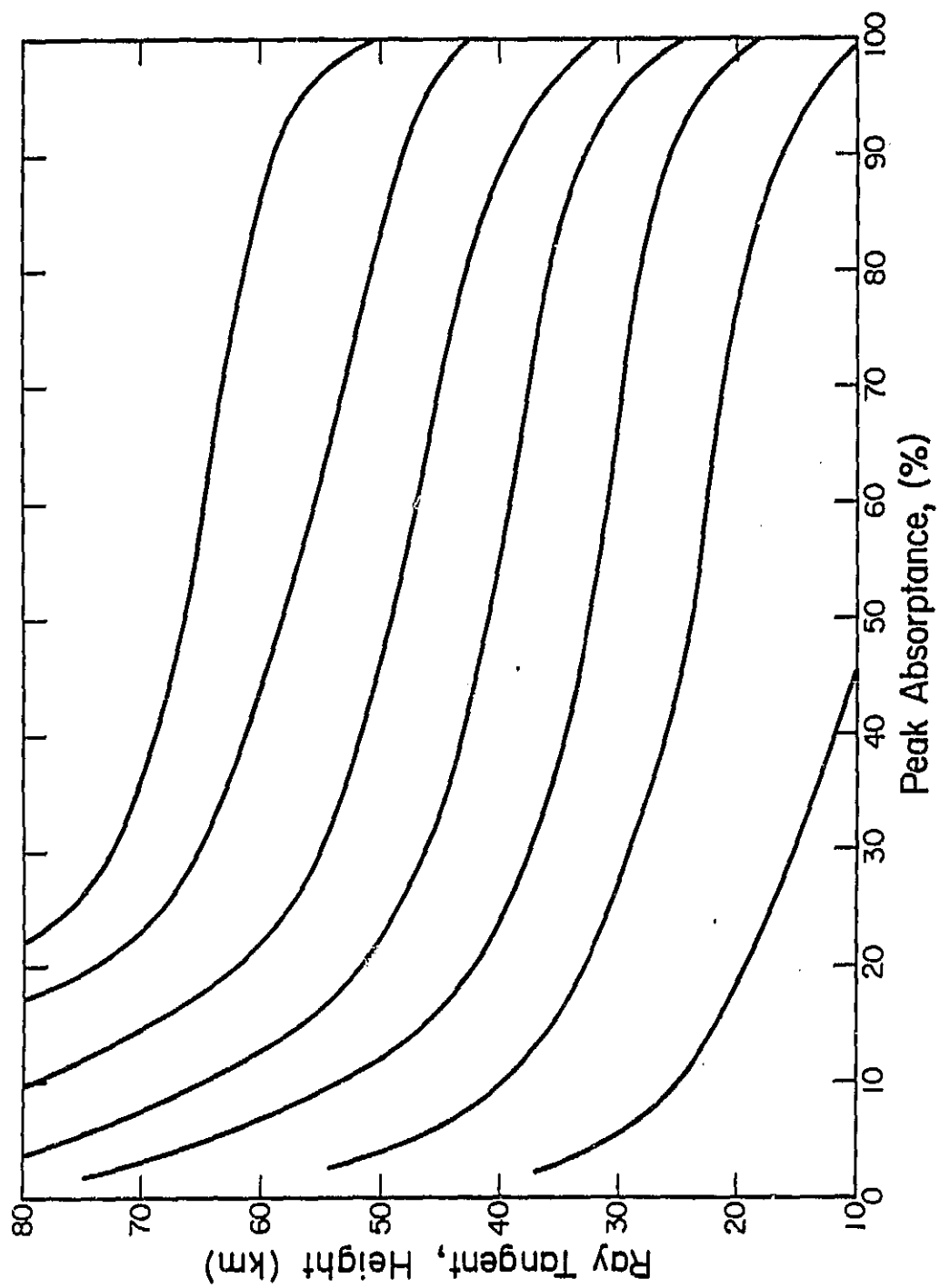


Fig. 3